



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 04:19 AM UTC

PDB ID : 6EB8 / pdb_00006eb8
Title : Crystal Structure of the Nipah Virus Phosphoprotein Multimerization Domain G519N
Authors : Bruhn, J.F.; Saphire, E.O.
Deposited on : 2018-08-06
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

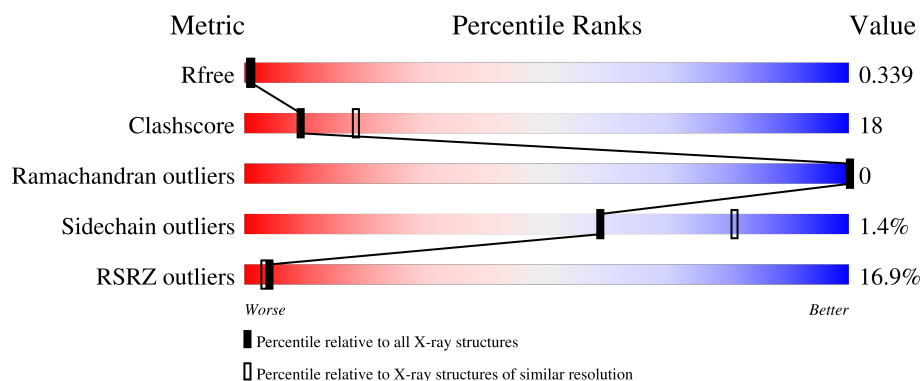
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



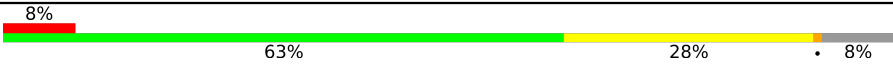
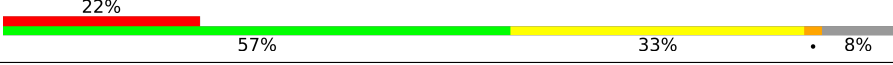
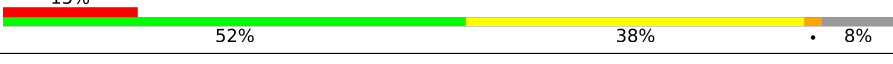
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	110	19% 55% 38% • 5%
1	B	110	16% 64% 27% 9%
1	C	110	15% 64% 27% 9%
1	D	110	18% 65% 25% • 8%
1	E	110	12% 59% 32% • 6%

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Mol	Chain	Length	Quality of chain
1	F	110	
1	G	110	
1	H	110	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6673 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Phosphoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	104	Total	C	N	O	S	0	0	0
			840	530	138	165	7			
1	E	103	Total	C	N	O	S	0	1	0
			838	529	138	164	7			
1	D	101	Total	C	N	O	S	0	0	0
			816	515	135	160	6			
1	C	100	Total	C	N	O	S	0	0	0
			807	509	133	159	6			
1	H	101	Total	C	N	O	S	0	0	0
			816	515	135	160	6			
1	F	101	Total	C	N	O	S	0	0	0
			816	515	135	160	6			
1	B	100	Total	C	N	O	S	0	0	0
			808	509	134	159	6			
1	G	101	Total	C	N	O	S	0	0	0
			816	515	135	160	6			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	469	SER	-	expression tag	UNP Q9IK91
A	519	ASN	GLY	engineered mutation	UNP Q9IK91
E	469	SER	-	expression tag	UNP Q9IK91
E	519	ASN	GLY	engineered mutation	UNP Q9IK91
D	469	SER	-	expression tag	UNP Q9IK91
D	519	ASN	GLY	engineered mutation	UNP Q9IK91
C	469	SER	-	expression tag	UNP Q9IK91
C	519	ASN	GLY	engineered mutation	UNP Q9IK91
H	469	SER	-	expression tag	UNP Q9IK91
H	519	ASN	GLY	engineered mutation	UNP Q9IK91
F	469	SER	-	expression tag	UNP Q9IK91
F	519	ASN	GLY	engineered mutation	UNP Q9IK91
B	469	SER	-	expression tag	UNP Q9IK91

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Chain	Residue	Modelled	Actual	Comment	Reference
B	519	ASN	GLY	engineered mutation	UNP Q9IK91
G	469	SER	-	expression tag	UNP Q9IK91
G	519	ASN	GLY	engineered mutation	UNP Q9IK91

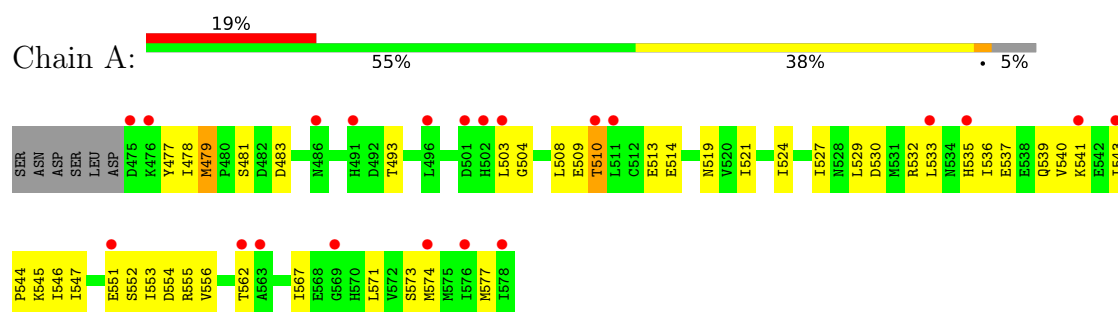
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	9	Total O 9 9	0	0
2	E	20	Total O 20 20	0	0
2	D	12	Total O 12 12	0	0
2	C	22	Total O 22 22	0	0
2	H	5	Total O 5 5	0	0
2	F	22	Total O 22 22	0	0
2	B	10	Total O 10 10	0	0
2	G	16	Total O 16 16	0	0

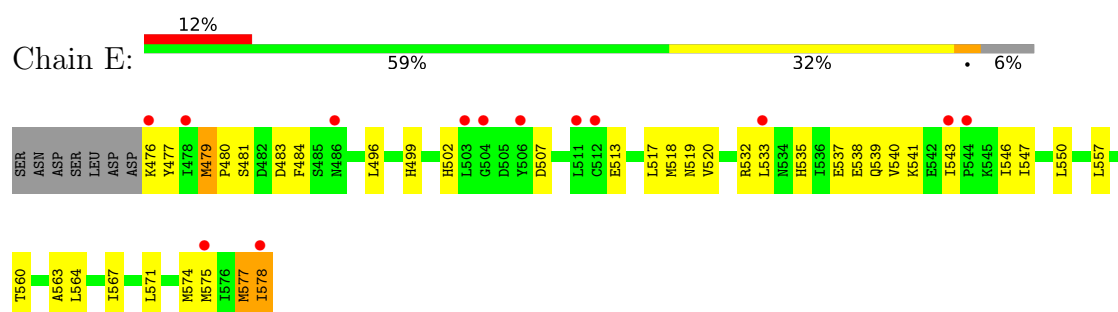
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

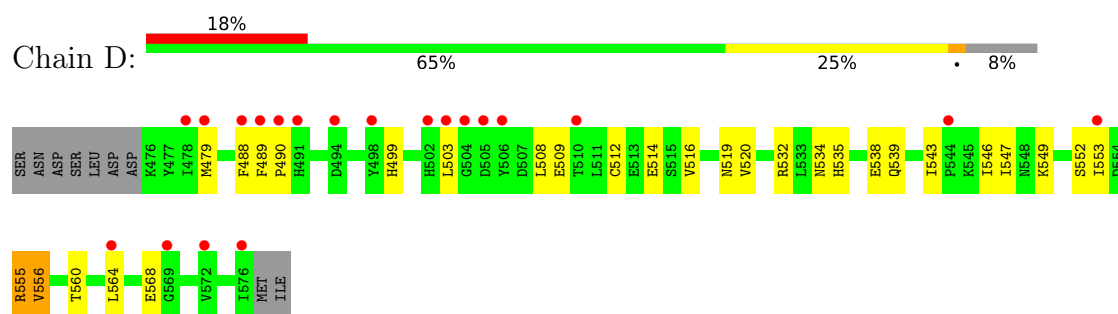
• Molecule 1: Phosphoprotein



• Molecule 1: Phosphoprotein

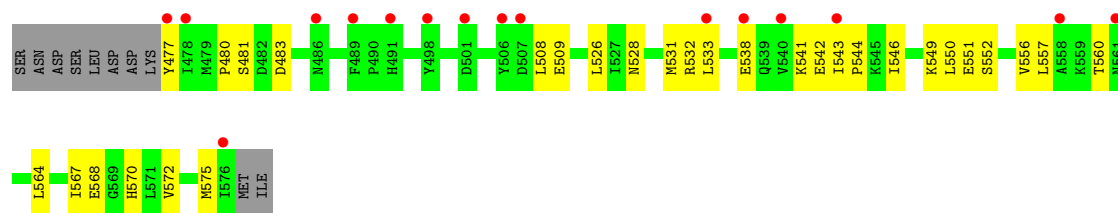


• Molecule 1: Phosphoprotein

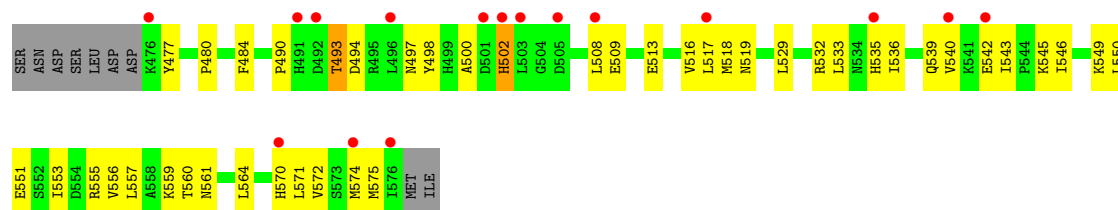


• Molecule 1: Phosphoprotein

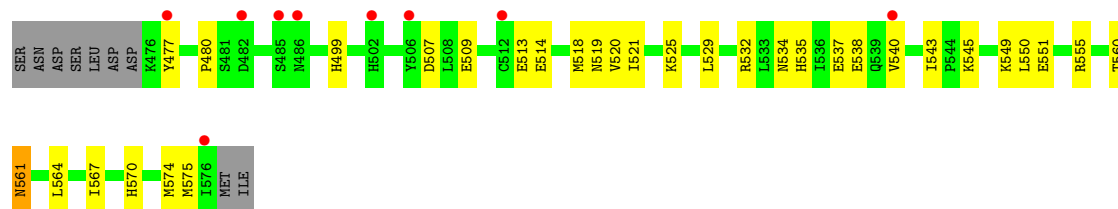




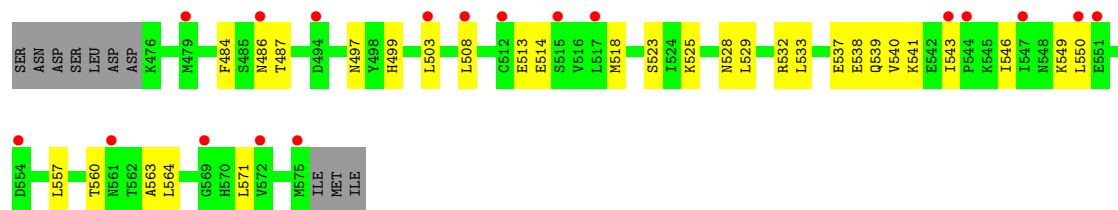
• Molecule 1: Phosphoprotein



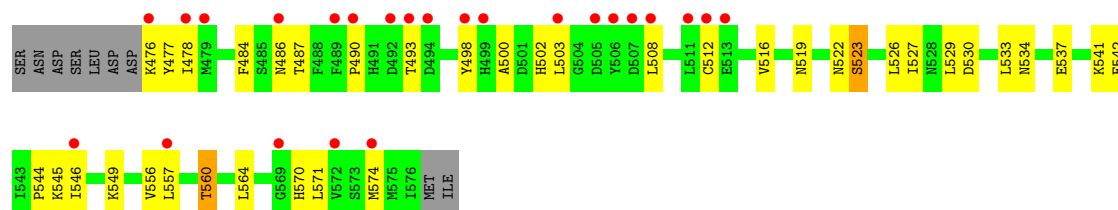
• Molecule 1: Phosphoprotein



• Molecule 1: Phosphoprotein



• Molecule 1: Phosphoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	48.00Å 76.62Å 80.54Å 100.46° 100.94° 108.05°	Depositor
Resolution (Å)	38.20 – 2.50 38.20 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.5 (38.20-2.50) 86.8 (38.20-2.50)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.65 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.276 , 0.338 0.276 , 0.339	Depositor DCC
R_{free} test set	1771 reflections (2.16%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.663	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 67.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	6673	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.42	0/853	0.68	0/1153
1	B	0.42	0/821	0.67	0/1110
1	C	0.45	0/820	0.70	0/1110
1	D	0.51	0/829	0.75	0/1121
1	E	0.54	0/851	0.76	1/1150 (0.1%)
1	F	0.50	0/829	0.75	0/1121
1	G	0.83	4/829 (0.5%)	0.76	0/1121
1	H	0.60	0/829	0.74	1/1121 (0.1%)
All	All	0.55	4/6661 (0.1%)	0.73	2/9007 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	522	ASN	C-O	-7.70	1.15	1.24
1	G	526	LEU	C-O	-7.67	1.15	1.24
1	G	523	SER	C-O	-6.26	1.16	1.24
1	G	527	ILE	C-O	-5.79	1.17	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	502	HIS	N-CA-C	5.88	121.50	113.97
1	E	577	MET	N-CA-C	5.18	116.92	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	840	0	836	43	0
1	B	808	0	801	29	0
1	C	807	0	799	33	0
1	D	816	0	812	39	1
1	E	838	0	836	57	1
1	F	816	0	812	47	0
1	G	816	0	812	53	0
1	H	816	0	812	57	0
2	A	9	0	0	1	0
2	B	10	0	0	1	0
2	C	22	0	0	1	0
2	D	12	0	0	0	0
2	E	20	0	0	0	0
2	F	22	0	0	1	0
2	G	16	0	0	1	0
2	H	5	0	0	1	0
All	All	6673	0	6520	237	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (237) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:508:LEU:HD22	1:G:508:LEU:CD1	1.56	1.34
1:H:508:LEU:CD2	1:G:508:LEU:HD13	1.71	1.20
1:H:508:LEU:HD22	1:G:508:LEU:HD13	1.14	1.08
1:F:525:LYS:NZ	1:G:523:SER:OG	1.87	1.08
1:H:508:LEU:CD2	1:G:508:LEU:CD1	2.35	1.02
1:H:508:LEU:HD22	1:G:508:LEU:HD11	1.42	1.00
1:E:560:THR:OG1	1:F:561:ASN:ND2	1.96	0.98
1:E:560:THR:HG1	1:F:561:ASN:ND2	1.68	0.91
1:E:541:LYS:HA	1:H:539:GLN:HE22	1.34	0.90
1:H:533:LEU:HD21	1:G:533:LEU:CD1	2.01	0.90
1:E:479:MET:HE2	1:F:514:GLU:HG3	1.53	0.89
1:H:533:LEU:HD21	1:G:533:LEU:HD12	1.53	0.89
1:E:479:MET:HE3	1:E:480:PRO:HD2	1.58	0.85
1:E:479:MET:HE3	1:E:480:PRO:CD	2.06	0.85
1:D:489:PHE:HB3	1:D:490:PRO:HD2	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:479:MET:CE	1:F:514:GLU:HG3	2.12	0.80
1:C:543:ILE:HD11	1:B:539:GLN:O	1.82	0.80
1:E:533:LEU:HD12	1:H:529:LEU:HD22	1.63	0.78
1:E:532:ARG:NH2	1:F:534:ASN:OD1	2.16	0.77
1:A:477:TYR:HE1	1:A:479:MET:HE3	1.50	0.77
1:F:560:THR:HG23	1:G:564:LEU:HD11	1.65	0.76
1:F:545:LYS:HG2	1:F:549:LYS:HE2	1.67	0.76
1:E:483:ASP:OD2	1:F:499:HIS:NE2	2.17	0.75
1:A:554:ASP:CG	1:D:549:LYS:HZ1	1.95	0.74
1:E:578:ILE:O	1:E:578:ILE:HG13	1.87	0.74
1:H:561:ASN:ND2	1:G:560:THR:OG1	2.14	0.74
1:G:476:LYS:HG3	1:G:477:TYR:H	1.53	0.74
1:G:498:TYR:O	1:G:502:HIS:ND1	2.21	0.72
1:H:533:LEU:CD2	1:G:533:LEU:HD12	2.20	0.72
1:E:479:MET:HE2	1:F:514:GLU:CG	2.19	0.71
1:C:549:LYS:NZ	2:C:601:HOH:O	2.23	0.71
1:E:476:LYS:HG3	1:E:477:TYR:H	1.55	0.71
1:H:498:TYR:O	1:H:502:HIS:ND1	2.24	0.70
1:D:489:PHE:HB3	1:D:490:PRO:CD	2.22	0.69
1:E:541:LYS:HA	1:H:539:GLN:NE2	2.06	0.69
1:D:499:HIS:O	1:D:503:LEU:HD22	1.92	0.67
1:E:479:MET:CE	1:E:480:PRO:HD2	2.23	0.67
1:A:574:MET:HA	1:A:577:MET:HE2	1.77	0.67
1:H:551:GLU:OE1	1:H:555:ARG:NH1	2.27	0.67
1:F:532:ARG:NH1	1:G:537:GLU:OE1	2.27	0.66
1:H:509:GLU:HA	1:G:508:LEU:HD21	1.78	0.65
1:H:542:GLU:OE1	1:H:545:LYS:HD2	1.96	0.65
1:A:508:LEU:H	1:A:508:LEU:HD12	1.61	0.64
1:H:533:LEU:HD21	1:G:533:LEU:HD11	1.80	0.64
1:H:559:LYS:NZ	2:H:602:HOH:O	2.26	0.64
1:H:556:VAL:O	1:H:560:THR:HG23	1.98	0.63
1:E:479:MET:HE3	1:E:480:PRO:HD3	1.80	0.63
1:H:571:LEU:HD13	1:G:570:HIS:HB2	1.80	0.63
1:A:552:SER:HA	1:A:555:ARG:HE	1.63	0.63
1:E:484:PHE:HB2	1:F:518:MET:HE1	1.80	0.62
1:C:564:LEU:HD11	1:B:560:THR:HG23	1.82	0.62
1:B:537:GLU:HA	1:B:540:VAL:HG22	1.80	0.62
1:E:574:MET:HE2	1:F:575:MET:CG	2.29	0.62
1:F:519:ASN:OD1	1:G:519:ASN:ND2	2.33	0.61
1:D:568:GLU:HG2	1:C:567:ILE:HG12	1.83	0.60
1:H:508:LEU:HD21	1:G:508:LEU:HD13	1.79	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:ILE:O	1:A:551:GLU:HG3	2.01	0.60
1:E:574:MET:HE2	1:F:575:MET:HG2	1.84	0.60
1:A:567:ILE:HD11	1:B:564:LEU:O	2.02	0.60
1:D:499:HIS:O	1:D:503:LEU:CD2	2.50	0.60
1:A:533:LEU:HD23	1:A:536:ILE:HB	1.85	0.59
1:D:509:GLU:HA	1:C:508:LEU:HD21	1.84	0.59
1:C:509:GLU:HG3	1:B:508:LEU:HD21	1.83	0.59
1:H:529:LEU:O	1:H:533:LEU:HD12	2.03	0.59
1:A:519:ASN:ND2	1:D:519:ASN:OD1	2.35	0.59
1:C:533:LEU:HD12	1:B:529:LEU:HD22	1.85	0.58
1:H:484:PHE:CZ	1:F:520:VAL:HG13	2.38	0.58
1:D:568:GLU:OE1	1:C:570:HIS:CD2	2.57	0.57
1:A:571:LEU:HG	1:B:571:LEU:HD11	1.86	0.57
1:A:529:LEU:HD22	1:B:533:LEU:HD12	1.86	0.57
1:D:512:CYS:O	1:D:516:VAL:HG23	2.06	0.56
1:A:544:PRO:HD3	1:D:539:GLN:OE1	2.05	0.56
1:C:557:LEU:HD21	1:B:557:LEU:HD21	1.86	0.56
1:D:503:LEU:HD22	1:D:503:LEU:N	2.21	0.56
1:F:525:LYS:NZ	1:G:523:SER:HG	2.01	0.56
1:E:479:MET:HE2	1:F:514:GLU:CD	2.30	0.56
1:A:537:GLU:O	1:A:541:LYS:HD3	2.05	0.55
1:F:507:ASP:HB2	2:F:605:HOH:O	2.07	0.55
1:A:481:SER:OG	1:B:514:GLU:OE2	2.24	0.55
1:A:554:ASP:OD2	1:D:549:LYS:NZ	2.34	0.54
1:E:537:GLU:HB2	1:H:536:ILE:HD11	1.89	0.54
1:B:538:GLU:O	1:B:541:LYS:HG2	2.08	0.54
1:D:499:HIS:NE2	1:C:483:ASP:OD2	2.41	0.54
1:G:512:CYS:O	1:G:516:VAL:HG23	2.08	0.53
1:C:552:SER:O	1:C:556:VAL:HG23	2.09	0.53
1:A:573:SER:O	1:A:577:MET:HG3	2.09	0.53
1:B:540:VAL:O	1:B:543:ILE:HD12	2.09	0.53
1:F:532:ARG:HD2	1:G:530:ASP:OD2	2.09	0.52
1:A:546:ILE:HG23	1:B:550:LEU:HD11	1.92	0.52
1:B:528:ASN:O	1:B:532:ARG:HD2	2.08	0.52
1:E:538:GLU:O	1:E:541:LYS:HG2	2.10	0.52
1:D:543:ILE:HG23	1:C:546:ILE:HD11	1.92	0.52
1:A:539:GLN:N	1:A:539:GLN:OE1	2.41	0.52
1:F:535:HIS:HA	1:F:538:GLU:HG3	1.91	0.52
1:E:520:VAL:HG13	1:G:484:PHE:CZ	2.45	0.51
1:A:521:ILE:HG23	1:D:488:PHE:CZ	2.45	0.51
1:B:497:ASN:HB2	2:B:602:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:503:LEU:HD22	1:D:503:LEU:H	1.75	0.51
1:B:486:ASN:OD1	1:B:487:THR:HG23	2.10	0.51
1:F:545:LYS:O	1:F:549:LYS:HG2	2.10	0.51
1:G:476:LYS:HG3	1:G:477:TYR:N	2.25	0.51
1:A:510:THR:HG23	1:D:479:MET:HE1	1.93	0.51
1:E:546:ILE:HD11	1:F:543:ILE:HG23	1.92	0.51
1:E:481:SER:HA	1:F:518:MET:HE2	1.93	0.51
1:G:529:LEU:O	1:G:533:LEU:HD13	2.11	0.51
1:D:514:GLU:OE1	1:C:481:SER:N	2.36	0.51
1:F:574:MET:HE1	1:G:574:MET:SD	2.51	0.51
1:E:575:MET:HG2	1:H:574:MET:HG3	1.93	0.50
1:A:546:ILE:HG23	1:B:550:LEU:CD1	2.41	0.50
1:D:520:VAL:HG13	1:B:484:PHE:CZ	2.47	0.50
1:F:545:LYS:HG2	1:F:549:LYS:CE	2.40	0.50
1:H:551:GLU:OE1	1:H:555:ARG:CZ	2.59	0.50
1:F:545:LYS:HE3	1:F:549:LYS:HE3	1.94	0.50
1:A:530:ASP:OD1	1:D:532:ARG:NE	2.44	0.50
1:A:540:VAL:HG12	1:D:539:GLN:HB2	1.94	0.50
1:E:537:GLU:OE1	1:H:535:HIS:ND1	2.45	0.50
1:D:534:ASN:OD1	1:C:532:ARG:NH2	2.35	0.49
1:A:536:ILE:HD11	1:B:537:GLU:HG3	1.94	0.49
1:E:563:ALA:HB1	1:F:564:LEU:HB3	1.94	0.49
1:C:543:ILE:CD1	1:B:539:GLN:O	2.59	0.49
1:C:528:ASN:HA	1:C:531:MET:HE2	1.94	0.49
1:E:499:HIS:CE1	1:H:480:PRO:HA	2.48	0.49
1:C:550:LEU:HD11	1:B:546:ILE:HG23	1.95	0.48
1:G:545:LYS:O	1:G:549:LYS:HG2	2.13	0.48
1:F:561:ASN:HD22	1:F:561:ASN:N	2.11	0.48
1:A:543:ILE:HG23	1:D:546:ILE:HD11	1.95	0.48
1:G:549:LYS:HA	1:G:549:LYS:HD3	1.62	0.48
1:A:533:LEU:HD23	1:A:533:LEU:HA	1.69	0.48
1:G:557:LEU:HA	1:G:560:THR:HB	1.95	0.47
1:H:493:THR:HG22	1:H:494:ASP:OD1	2.15	0.47
1:E:574:MET:HE2	1:F:575:MET:HG3	1.95	0.47
1:D:568:GLU:OE1	1:C:570:HIS:HD2	1.96	0.47
1:A:553:ILE:HA	1:A:556:VAL:HG12	1.95	0.47
1:H:555:ARG:O	1:H:559:LYS:HG3	2.15	0.47
1:D:556:VAL:O	1:D:560:THR:OG1	2.28	0.47
1:A:509:GLU:HA	1:D:508:LEU:HD21	1.97	0.46
1:E:520:VAL:HG13	1:G:484:PHE:CE2	2.50	0.46
1:E:543:ILE:O	1:E:547:ILE:HD12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:570:HIS:O	1:G:574:MET:HG2	2.15	0.46
1:F:532:ARG:HH12	1:G:537:GLU:CD	2.23	0.46
1:C:551:GLU:HG3	1:B:549:LYS:NZ	2.31	0.46
1:H:517:LEU:HD21	1:G:500:ALA:HA	1.97	0.46
1:E:571:LEU:HD21	1:H:570:HIS:HB2	1.97	0.46
1:G:541:LYS:O	1:G:541:LYS:HG2	2.15	0.46
1:H:549:LYS:HA	1:H:549:LYS:HD3	1.63	0.46
1:H:572:VAL:HA	1:H:575:MET:HE2	1.98	0.46
1:B:499:HIS:O	1:B:503:LEU:HG	2.16	0.45
1:D:549:LYS:HE2	1:D:553:ILE:HG13	1.98	0.45
1:C:541:LYS:O	1:C:541:LYS:HG2	2.16	0.45
1:F:570:HIS:HB2	1:G:571:LEU:HD13	1.97	0.45
1:C:477:TYR:OH	1:C:480:PRO:HD3	2.16	0.45
1:D:535:HIS:O	1:D:538:GLU:HG2	2.16	0.45
1:A:535:HIS:O	1:A:539:GLN:OE1	2.35	0.44
1:H:557:LEU:HB3	1:G:556:VAL:HG11	1.99	0.44
1:B:518:MET:HE3	1:B:518:MET:HB3	1.79	0.44
1:G:560:THR:O	1:G:564:LEU:HG	2.17	0.44
1:A:552:SER:OG	1:A:555:ARG:NH2	2.50	0.44
1:D:499:HIS:ND1	1:C:480:PRO:HG3	2.33	0.44
1:E:517:LEU:HD21	1:H:500:ALA:HA	1.98	0.44
1:H:549:LYS:O	1:H:553:ILE:HD12	2.18	0.44
1:H:540:VAL:HG13	1:H:543:ILE:HD12	2.00	0.44
1:E:499:HIS:ND1	1:H:480:PRO:HG3	2.32	0.44
1:A:478:ILE:HG22	1:A:483:ASP:HB2	1.99	0.43
1:A:521:ILE:HG23	1:D:488:PHE:HZ	1.82	0.43
1:E:479:MET:HE1	1:F:514:GLU:HG3	1.98	0.43
1:E:575:MET:HG2	1:H:574:MET:CG	2.48	0.43
1:E:535:HIS:O	1:E:539:GLN:HG3	2.18	0.43
1:D:489:PHE:CB	1:D:490:PRO:CD	2.92	0.43
1:F:532:ARG:NH2	1:G:534:ASN:OD1	2.51	0.43
1:E:507:ASP:OD1	1:E:507:ASP:N	2.50	0.43
1:F:567:ILE:HG23	1:G:571:LEU:HD11	1.99	0.43
1:E:496:LEU:HD13	1:F:521:ILE:HG13	2.01	0.43
1:E:550:LEU:HD11	1:H:546:ILE:HG23	2.00	0.43
1:E:502:HIS:HB2	1:H:477:TYR:CE1	2.53	0.43
1:A:532:ARG:O	1:A:536:ILE:N	2.39	0.43
1:H:490:PRO:HA	1:H:493:THR:HB	2.00	0.43
1:E:537:GLU:OE2	1:H:532:ARG:HD3	2.19	0.42
1:D:547:ILE:CD1	1:C:542:GLU:HB3	2.49	0.42
1:F:529:LEU:HD22	1:G:533:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:480:PRO:C	1:F:518:MET:HE3	2.44	0.42
1:H:498:TYR:CE2	1:G:478:ILE:HG12	2.53	0.42
1:C:564:LEU:HD13	1:B:563:ALA:HB3	2.00	0.42
1:F:477:TYR:OH	1:F:480:PRO:HD3	2.18	0.42
1:F:550:LEU:HD23	1:F:550:LEU:HA	1.83	0.42
1:A:493:THR:HG22	2:A:606:HOH:O	2.18	0.42
1:G:541:LYS:O	1:G:544:PRO:HD2	2.19	0.42
1:D:564:LEU:HD11	1:C:560:THR:HG23	2.02	0.42
1:H:513:GLU:HA	1:H:516:VAL:HG12	2.02	0.42
1:H:519:ASN:ND2	1:G:519:ASN:OD1	2.53	0.42
1:E:537:GLU:HA	1:H:536:ILE:HG12	2.02	0.42
1:C:543:ILE:HG13	1:C:544:PRO:HD3	2.02	0.42
1:D:499:HIS:C	1:D:503:LEU:CD2	2.92	0.42
1:F:537:GLU:HA	1:F:540:VAL:HG22	2.01	0.42
1:A:513:GLU:HG3	1:D:503:LEU:HB2	2.01	0.41
1:E:567:ILE:HD11	1:F:564:LEU:O	2.20	0.41
1:A:532:ARG:HA	1:A:535:HIS:HB3	2.02	0.41
1:A:545:LYS:HE2	1:A:545:LYS:HB2	1.89	0.41
1:C:480:PRO:HA	1:C:483:ASP:HB3	2.01	0.41
1:C:526:LEU:HD13	1:B:525:LYS:HB2	2.02	0.41
1:C:568:GLU:O	1:C:572:VAL:HG23	2.20	0.41
1:C:557:LEU:CD2	1:B:557:LEU:HD21	2.51	0.41
1:F:509:GLU:O	1:F:513:GLU:HB2	2.21	0.41
1:G:490:PRO:HA	1:G:493:THR:HB	2.01	0.41
1:E:480:PRO:CB	1:F:518:MET:HE3	2.50	0.41
1:H:516:VAL:CG1	1:G:503:LEU:HD13	2.51	0.41
1:G:542:GLU:HA	1:G:545:LYS:HD2	2.01	0.41
1:E:543:ILE:HG22	1:E:547:ILE:CD1	2.51	0.41
1:H:497:ASN:HA	1:H:500:ALA:HB3	2.02	0.41
1:A:514:GLU:OE2	1:D:479:MET:HE3	2.20	0.41
1:E:518:MET:HE3	1:E:518:MET:HB3	1.98	0.41
1:E:540:VAL:O	1:H:539:GLN:NE2	2.54	0.41
1:E:564:LEU:HD21	1:H:564:LEU:CD2	2.50	0.41
1:E:513:GLU:O	1:E:517:LEU:HD12	2.21	0.41
1:E:557:LEU:CD1	1:H:553:ILE:HG23	2.51	0.41
1:H:551:GLU:OE2	1:G:549:LYS:NZ	2.43	0.41
1:A:504:GLY:HA2	1:B:513:GLU:OE2	2.21	0.41
1:E:476:LYS:CG	1:E:477:TYR:H	2.31	0.41
1:C:572:VAL:HA	1:C:575:MET:HE3	2.03	0.41
1:G:477:TYR:HE2	2:G:615:HOH:O	2.04	0.41
1:E:546:ILE:HG23	1:F:550:LEU:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:552:SER:HA	1:D:555:ARG:HD2	2.03	0.41
1:D:568:GLU:HG2	1:C:567:ILE:CG1	2.49	0.41
1:C:538:GLU:HA	1:C:541:LYS:CB	2.51	0.40
1:G:486:ASN:OD1	1:G:487:THR:HG23	2.21	0.40
1:G:508:LEU:HA	1:G:508:LEU:HD23	1.87	0.40
1:A:552:SER:HA	1:A:555:ARG:NE	2.34	0.40
1:H:508:LEU:HD23	1:G:508:LEU:CD2	2.50	0.40
1:F:551:GLU:HB3	1:F:555:ARG:HH21	1.86	0.40
1:B:557:LEU:HA	1:B:557:LEU:HD23	1.89	0.40
1:E:557:LEU:HA	1:E:557:LEU:HD23	1.88	0.40
1:H:550:LEU:HD11	1:G:546:ILE:HG23	2.03	0.40
1:G:542:GLU:O	1:G:545:LYS:HB2	2.22	0.40
1:A:553:ILE:O	1:A:556:VAL:HG12	2.22	0.40
1:A:503:LEU:HD23	1:A:503:LEU:HA	1.67	0.40
1:A:524:ILE:HA	1:A:527:ILE:HD12	2.04	0.40
1:E:519:ASN:HB3	1:H:518:MET:HB3	2.02	0.40
1:F:564:LEU:HD23	1:F:564:LEU:HA	1.94	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:577:MET:O	1:D:555:ARG:NH1[1_446]	1.68	0.52

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	102/110 (93%)	101 (99%)	1 (1%)	0	100	100
1	B	98/110 (89%)	98 (100%)	0	0	100	100
1	C	98/110 (89%)	96 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	99/110 (90%)	97 (98%)	2 (2%)	0	100	100
1	E	102/110 (93%)	100 (98%)	2 (2%)	0	100	100
1	F	99/110 (90%)	99 (100%)	0	0	100	100
1	G	99/110 (90%)	99 (100%)	0	0	100	100
1	H	99/110 (90%)	96 (97%)	3 (3%)	0	100	100
All	All	796/880 (90%)	786 (99%)	10 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	99/105 (94%)	96 (97%)	3 (3%)	36	64
1	B	95/105 (90%)	94 (99%)	1 (1%)	65	84
1	C	95/105 (90%)	95 (100%)	0	100	100
1	D	96/105 (91%)	94 (98%)	2 (2%)	47	74
1	E	99/105 (94%)	97 (98%)	2 (2%)	48	75
1	F	96/105 (91%)	95 (99%)	1 (1%)	68	86
1	G	96/105 (91%)	95 (99%)	1 (1%)	68	86
1	H	96/105 (91%)	95 (99%)	1 (1%)	68	86
All	All	772/840 (92%)	761 (99%)	11 (1%)	59	81

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	479	MET
1	A	510	THR
1	A	562	THR
1	E	479	MET
1	E	578	ILE

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Mol	Chain	Res	Type
1	D	555	ARG
1	D	556	VAL
1	H	493	THR
1	F	561	ASN
1	B	523	SER
1	G	560	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	534	ASN
1	E	519	ASN
1	C	539	GLN
1	C	570	HIS
1	H	539	GLN
1	H	561	ASN
1	F	491	HIS
1	F	561	ASN
1	G	570	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	104/110 (94%)	1.30	21 (20%) 3 2	21, 45, 56, 65	0
1	B	100/110 (90%)	1.24	18 (18%) 3 3	26, 42, 56, 68	0
1	C	100/110 (90%)	1.21	16 (16%) 5 4	24, 41, 56, 60	0
1	D	101/110 (91%)	1.35	20 (19%) 3 2	19, 46, 59, 65	0
1	E	103/110 (93%)	1.09	13 (12%) 8 6	20, 40, 54, 63	1 (0%)
1	F	101/110 (91%)	1.07	9 (8%) 15 13	26, 39, 51, 59	0
1	G	101/110 (91%)	1.39	24 (23%) 2 1	23, 47, 58, 73	0
1	H	101/110 (91%)	1.39	16 (15%) 5 4	29, 43, 56, 75	0
All	All	811/880 (92%)	1.25	137 (16%) 4 3	19, 43, 57, 75	1 (0%)

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	501	ASP	6.0
1	H	496	LEU	4.9
1	D	488	PHE	4.2
1	C	477	TYR	3.9
1	D	576	ILE	3.9
1	H	576	ILE	3.9
1	D	506	TYR	3.8
1	D	478	ILE	3.8
1	B	512	CYS	3.7
1	D	479	MET	3.7
1	A	510	THR	3.6
1	G	503	LEU	3.6
1	C	576	ILE	3.6
1	D	489	PHE	3.5
1	B	550	LEU	3.5
1	A	576	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	G	478	ILE	3.5
1	B	494	ASP	3.5
1	B	486	ASN	3.4
1	G	486	ASN	3.3
1	H	492	ASP	3.3
1	E	478	ILE	3.2
1	C	486	ASN	3.1
1	G	493	THR	3.1
1	G	569	GLY	3.1
1	G	489	PHE	3.0
1	A	476	LYS	3.0
1	A	578	ILE	3.0
1	G	498	TYR	3.0
1	G	508	LEU	3.0
1	F	485	SER	3.0
1	F	486	ASN	3.0
1	C	507	ASP	3.0
1	E	543	ILE	2.9
1	E	476	LYS	2.9
1	G	479	MET	2.9
1	A	562	THR	2.9
1	G	506	TYR	2.9
1	A	563	ALA	2.8
1	B	561	ASN	2.8
1	C	558	ALA	2.8
1	H	574	MET	2.8
1	F	512	CYS	2.8
1	E	503	LEU	2.7
1	C	538	GLU	2.7
1	D	494	ASP	2.7
1	H	501	ASP	2.7
1	F	477	TYR	2.7
1	H	570	HIS	2.7
1	D	490	PRO	2.7
1	B	572	VAL	2.7
1	B	551	GLU	2.7
1	B	554	ASP	2.6
1	D	572	VAL	2.6
1	E	506	TYR	2.6
1	H	502	HIS	2.6
1	C	498	TYR	2.6
1	C	478	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	540	VAL	2.6
1	F	502	HIS	2.6
1	C	501	ASP	2.6
1	B	569	GLY	2.6
1	D	491	HIS	2.6
1	G	507	ASP	2.5
1	C	561	ASN	2.5
1	F	540	VAL	2.5
1	B	544	PRO	2.5
1	A	496	LEU	2.5
1	H	491	HIS	2.5
1	E	578	ILE	2.4
1	D	503	LEU	2.4
1	G	572	VAL	2.4
1	G	574	MET	2.4
1	G	513	GLU	2.4
1	H	508	LEU	2.4
1	G	511	LEU	2.4
1	G	476	LYS	2.4
1	A	569	GLY	2.4
1	A	503	LEU	2.4
1	G	494	ASP	2.4
1	B	575	MET	2.4
1	C	543	ILE	2.3
1	B	503	LEU	2.3
1	A	502	HIS	2.3
1	A	543	ILE	2.3
1	D	505	ASP	2.3
1	G	492	ASP	2.3
1	C	489	PHE	2.3
1	C	506	TYR	2.3
1	E	544	PRO	2.3
1	D	544	PRO	2.3
1	F	482	ASP	2.3
1	A	541	LYS	2.3
1	H	540	VAL	2.3
1	H	535	HIS	2.3
1	H	517	LEU	2.3
1	D	502	HIS	2.2
1	E	511	LEU	2.2
1	D	564	LEU	2.2
1	G	505	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	506	TYR	2.2
1	D	510	THR	2.2
1	F	576	ILE	2.2
1	B	543	ILE	2.2
1	B	547	ILE	2.2
1	G	546	ILE	2.2
1	A	486	ASN	2.2
1	A	535	HIS	2.2
1	E	504	GLY	2.2
1	A	475	ASP	2.2
1	E	512	CYS	2.2
1	D	504	GLY	2.2
1	H	503	LEU	2.2
1	G	512	CYS	2.2
1	A	491	HIS	2.1
1	A	511	LEU	2.1
1	D	569	GLY	2.1
1	C	533	LEU	2.1
1	B	479	MET	2.1
1	E	533	LEU	2.1
1	A	551	GLU	2.1
1	H	505	ASP	2.1
1	A	574	MET	2.1
1	A	533	LEU	2.0
1	B	508	LEU	2.0
1	B	517	LEU	2.0
1	H	542	GLU	2.0
1	H	476	LYS	2.0
1	D	498	TYR	2.0
1	G	499	HIS	2.0
1	G	557	LEU	2.0
1	E	486	ASN	2.0
1	D	553	ILE	2.0
1	E	575	MET	2.0
1	G	490	PRO	2.0
1	C	491	HIS	2.0
1	B	515	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.